Hydrogen cyanide 74-90-8 | DTXSID9024148

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 14.5 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.40e-01

Confidence level: 6.65e-01

Nearest Neighbors from the Training Set

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Hydrogen cyanide Measured: 37.0 Predicted: 14.5 Image not found

Potassium cyanide Measured: 11.1 Predicted: 14.5 Image not found

Acetonitrile
Measured: 24.4
Predicted: 8.60

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Acrylonitrile
Measured: 1.40
Predicted: 1.84

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Chloroacetonitrile Measured: 1.32 Predicted: 1.82